Accelerating Advanced Energy Materials Discovery with AI and Modern Characterization Tools

Maria C. Asensio

Materials Science Institute of Madrid (ICMM/CSIC), Cantoblanco, E-28049 Madrid, SPAIN
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MATINÉE, CSIC Associated Unit between ICMM and the Materials Science of the University of Valencia (ICMUV), Madrid, SPAIN

Materials innovation is central to advancing clean energy technologies—powering breakthroughs in batteries, solar cells, low-energy semiconductors, thermal storage, and carbon capture and conversion. However, the discovery and development of new materials remain a major bottleneck, typically requiring 10 to 20 years of costly and time-consuming research. This challenge stems from the vastness of chemical space and the need for exhaustive characterization at sub-micrometre and atomic scales.

In this presentation, I will introduce a synergistic approach that integrates experimental techniques with artificial intelligence (AI) to accelerate the discovery and optimization of advanced energy materials. I will showcase recent AI-driven methods, aligned with the goals of the Materials Genome Initiative [1], for predicting novel materials with tailored properties. This includes a deep learning framework based on graph neural networks (GNNs), trained on extensive datasets—such as those from the Materials Project, NOMAD, and other large-scale repositories—to identify promising candidates for energy storage applications.

Predicted materials are validated through advanced characterization techniques, including synchrotron radiation and neutron-based methods. I will present also recent findings using Nano Angle-Resolved Photoelectron Spectroscopy (Nano-ARPES), a powerful k-space nanoscope that enables high-resolution, momentum-resolved mapping of electronic band structures at the nano- and mesoscales hat provide the electronic finger print of complex materilas. This technique offers insights into how nanoscale heterogeneities and confinement effects influence valence band electronic states near the Fermi level [2–6].

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